



Sandia National Laboratories'

Organic Materials Program



Sandia

Sandia National Laboratories' Organic Materials Program

Sandia National Laboratories has developed large and highly productive capabilities in the science and technology of polymers and other organic materials. Our customer base, originally developed and supported exclusively by the nation's Nuclear Weapons Complex, now includes a number of DOE and DoD offices, other federal agencies, and a large number of commercial companies. Sandia has earned a reputation for technical excellence and strong partnering relationships.

SCIENTIFIC CAPABILITIES

Synthesis and Processing

Sandia has developed the technical base to support internal and external customers requiring novel materials for specialized applications, such as replacements for materials no longer available or considered environmentally unacceptable.

Recent applications include chemical transducers for specialized sensors, catalysts, foams and other porous materials for high-surface-area applications, and a variety of "smart materials" designed to respond to specific stimuli.

Modeling and Simulation

Sandia extensively draws upon its models and computer simulations to produce important applications that include:

- predictions of materials properties to guide the choice of molecular structures for laboratory synthesis
- guides for optimizing materials properties, component designs, and manufacturing processes
- predictions of effective service life and failure modes

Recent applications include:

- predictions of polymer-blend miscibility
- nonlinear viscoelasticity under extreme conditions
- catalysis optimization

Aging and Reliability

Sandia scientists are internationally recognized for their contributions to the fundamental understanding of the aging mechanism in polymeric materials in thermal, radiation, photo, and combined environments. Our experts have developed unique characterization tools for measuring, with high spatial resolution and extreme sensitivity, the physical and chemical aspects of aging.

This expertise, combined with Sandia modeling and synthesis capabilities, enables us to measure the real-time aging of polymers under ambient conditions, predict materials failure under use conditions for a wide variety of applications, and implement means for lifetime extension.

Sandia's organic and polymeric science and technology program is among the largest in the world. Coupled with our systems engineering expertise, Sandia brings an unparalleled breadth of insight and capability to polymer science and engineering problems.

More than one hundred successful Cooperative Research and Development Agreements (CRADAs) attest to our ability to deliver unique solutions to challenging problems.

Supercritical and Subcritical CO₂ Processing

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Sandia has developed supercritical/subcritical carbon dioxide (SCCO₂) processing, which can be applied to materials and process development.

SCCO₂ —

- Possesses liquid-like densities and solvating properties.
- Functions as a good solvent for nonpolar organic compounds.
- Exhibits gas-like transport properties of viscosity and diffusivity along with negligible surface tension similar to a gas.

This combination of properties allows the supercritical fluid to access very small, complicated geometries to dissolve and remove organic contaminants. Sandia has extraction vessels of 1 to 20 liters, supercritical fluid chromatograph/extraction devices, and optical view cells for studying the solubility and phase phenomena in supercritical fluids.

Applications

- Particulate-free cleaning process for the semiconductor industry.
- Stiction elimination through the use of nonaqueous processing/cleaning solutions.
- Micromachined polysilicon microelectromechanical device processing.

Potential Benefits

- Elimination of surface tension effects and subsequent sticking of polysilicon structures to the silicon wafer substrate when using conventional air drying.

- Readily accessible, ~1-3 micron spaces between microstructures.
- Substitution of supercritical CO₂ for toxic or ozone-depleting cleaning solvents in extraction, cleaning, and other applications.
- Reduction in hazardous waste disposal associated with the above.

Demonstrated Achievements

- Successfully applied supercritical CO₂ extraction technology to extract capillary fluids from polysilicon micromechanical devices in Sandia's Class 1 Microelectronic Development Facility.
- Contributed to the development of "Superscrub" line of supercritical CO₂ extraction products sold by Autoclave Engineers.
- Designed supercritical CO₂ recyclable cleaning facility at a large government contractor under a joint DOE, DoD/USAF program.

References

- 1995 DOE Office of Industrial Technologies award for successful commercialization of supercritical CO₂ cleaning technology.
- Invited presentations at ACS, AIChE, Materials Research, SAMPE, and SPIE societies.
- Technical papers on supercritical fluid research published in *Journal of Supercritical Fluids* and *Chemistry of Materials*.

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Microcellular Materials

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Sandia National Laboratories offers specialized expertise in polymer chemistry and macromolecular physics across a wide range of materials applications to yield microcellular materials and their derivatives, engineered to provide unique performance advantages.

Sandia's computational tools use proprietary code developed to predict performance (adsorption and transport of two-phase media) in microcellular materials.

Applications

- Energy storage materials devices.
- Filtration and separation.
- Insulation media.
- Low-mass structures.
- Low-temperature alloys via non-abruting methods.
- Powders with unique shapes and properties.
- Stable suspensions for biomedical.
- Low-density foams for immobilizing particulate beds.

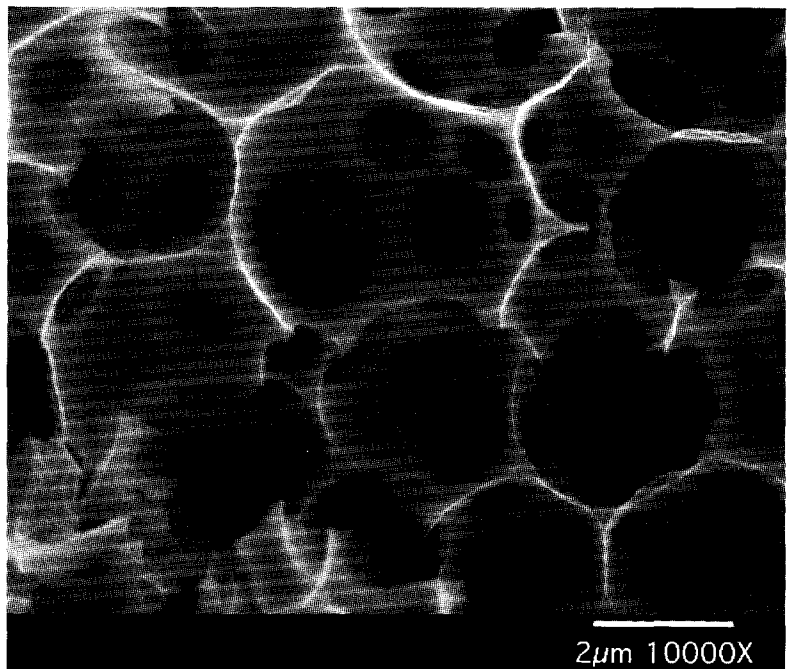
Potential Benefits

- Developing specific engineered products in lieu of adapting existing products for new applications.
- Custom tailoring of properties such as cell size, window size, and composition.

Demonstrated Achievements

- Completion of more than 50 man-years of experience in the synthesis of critical new materials of nonnuclear components.
- Transfer of two recent Sandia inventions into the commercial sector within 16 months of conception.
- Introduction of four products into the market by two different Fortune 100 companies (including Bethlehem Advanced Materials Corp.) using Sandia's microcellular expertise as an enabling technology in cost-effective solutions for value-added products.

Carbon



**2-3 μm macroporosity @ 20 m²/gr
< 100Å microporosity @ 500 m²/gr**

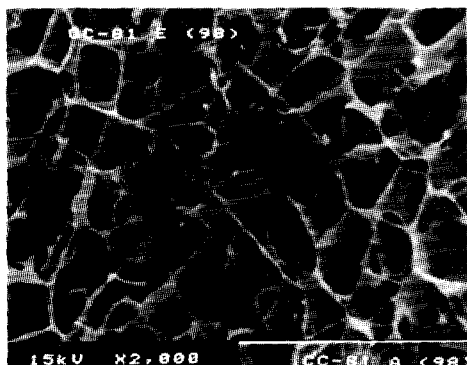


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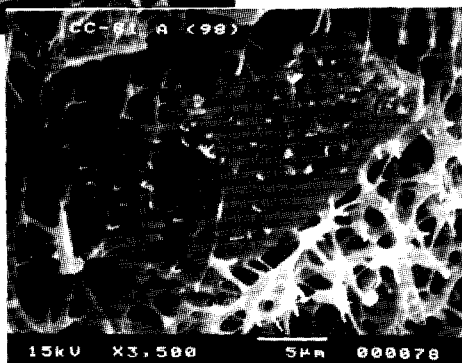


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**Polymeric
Microcellular
Foams**

**Particulate beds
immobilized
with microcellular
foams**



References

- Five patents issued with 3-4 disclosures being pursued.
- Several Cooperative Research and Development Agreements (CRADAs) and partnerships.
- Publications in MRS, ECS, and ACS proceedings.
- University, industry, and national lab alliances.

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Organic Coatings with Tailored Properties

Organic Materials Program

Organic coatings with a wide range of tailored properties can be developed through Sandia's expertise in the following areas:

- ROMP polymerization of functionalized block copolymers
- Conventional coupling agents
- Organic/inorganic multilayer films
- Plasma deposited/grafted films
- Liquid crystal thin films
- Gradient thin films
- Dye containing thin films

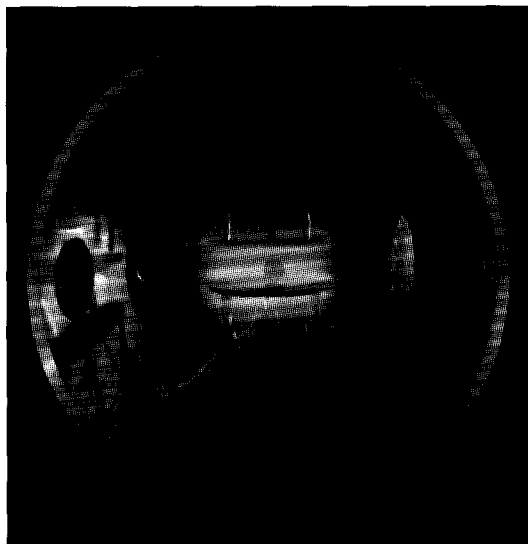
Targeted properties include adhesion, corrosion resistance, lubrication, wear, optical, and electronic. Sandia has developed a suite of specialized techniques for characterizing structure and properties of organic thin films and coatings, including neutron and X-ray reflection.

Applications

- Electronic packaging.
- Aerospace.
- Automotive.

Potential Benefits

Chemistry, structure, and mechanical properties are all interrelated capabilities required for effective and productive organic coating development.



There is no single approach to developing novel organic coatings. However, applying Sandia's diverse capabilities to the development of organic coatings with tailored properties increases the odds over a conventional single-path approach for developing a successful new product.

Demonstrated Achievements

- Synthesis and application of functionalized block copolymer films tailored for adhesion, including specialized capacitors, sensors, and adhesion promoters.
- Five-year collaborative agreement to develop silane coupling agents for the tire and printed wiring board industries.
- Optical thin films, liquid crystals, and gradient thin films.

References

- Two patents issued and one patent pending.
- Publications in *Journal of Material Science*, *Materials Research Society Symposium Process*, *Journal of Adhesion*, *Journal of Chem. Physics*, *Macromolecules*, *Physics Review Letters*.

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Modeling and Simulation

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Sandia possesses the most extensive modeling and simulation capabilities found anywhere in the world. These capabilities have been applied to the technology of polymers and other organic materials to meet the critical needs of federal customers and a diverse clientele of U. S. industries. Important applications include:

- Predictions of materials properties to guide the choice of molecular structures for laboratory synthesis,
- Guides for optimizing materials properties, component designs, and manufacturing processes, and
- Predictions of effective service life and failure modes.

Starting at the molecular level, Sandia's simulation modeling capabilities have been applied to polymeric materials to produce desired properties. These models are made possible with massively parallel computers, which minimize expensive and time-consuming laboratory experiments, while simultaneously developing a more accurate understanding of cause-and-effect relationships between chemical structure and final properties.

Modelers employ Polymer Reference Interaction Site Model (PRISM) modeling capabilities to design new polymer alloys and blends from the knowledge gained at the molecular level. These specific modeling and simulation capabilities are called:

- Molecular Simulation of Polymeric Materials
- Computer Modeling of Polymeric Materials

Sandia has specific experience in applying its powerful and unique modeling capabilities to the organic sciences and polymer technologies to enhance understanding and develop

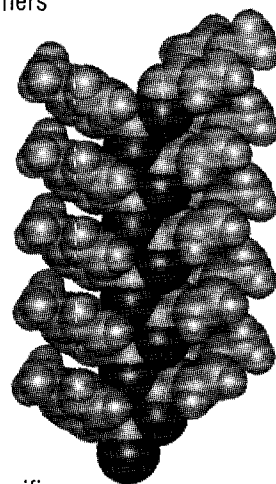
materials used in electronic components.

Specific materials applications include thermoset and particle-reinforced polymers plus electronic packaging and flip chip underfill. These process modeling capabilities are based on proprietary code and use the same massively parallel computers found only at Sandia.

Sandia has extended its modeling capabilities to develop an understanding of the dynamics of underfill flow and adhesion properties. These specific modeling and aging/reliability capabilities are called:

- Modeling and Predicting Stresses in Thermoset Materials
- Modeling Particle-Reinforced Polymers
- Flip Chip Underfill Studies
- Adhesion Studies

Each of these proprietary Sandia capabilities may be applied separately or in combination to solve challenging problems in the field of polymer and other organic sciences. Sandia has the flexibility to form specific teams of technical experts from any or all of the above capabilities to focus expertise on specific technical challenges.



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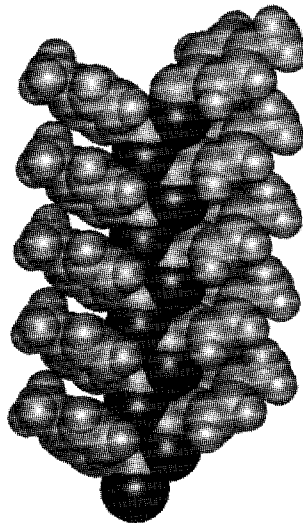
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Modeling Particle-Reinforced Polymers

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Sandia National Laboratories offers specialized expertise in

- Unique materials knowledge, computer codes, and flow modeling applied to the experimental characterization and modeling flow of particle polymers into complicated molds, including particle-migration phenomena.
- Specialized microscopy and X-ray/neutron scattering for characterizing particle micro-structure.
- State-of-the-art equipment for characterizing fluid rheological properties.
- Computational facilities, including Intel Paragon and massively parallel teraflops computer.
- Proprietary and unique fluid-flow analysis codes.



Applications

- Flip-chip encapsulation via capillary underflow of highly filled polymers.
- Inexpensive injection-molded parts, such as plastic trays that hold a group of chips in precise dimensional register during high-speed automated processing (this level of dimensional stability requires uniform thermal expansion, which requires uniform distribution of particles).
- Coatings.
- Development of code for modeling injected-molded polymers and for materials of particle-imbedded polyimides used for interlayer dielectric in IC and PWB.

Potential Benefits

- Improved quality by reducing voids caused by nonuniform flow and migration of particles that cause defects initiating cracking and delamination.
- Reduced cost of building expensive prototypes (of PC chips, for example) by doing computational modeling of a key production process.

Demonstrated Achievements

Particle structure characterization, computational modeling, and flow visualization on a 40-micron, glass-particle-reinforced epoxy encapsulant.

References

- One U.S. patent.
- Eighteen publications in refereed journals, including *Journal of Rheology*, *Journal of Fluid Mechanics*, and *Journal of Computational Mechanics*.
- Contribution to more than one dozen book chapters and international conference proceedings.
- Peer-reviewed publications on experimental and computational analysis of particle reinforced fluid rheology.
- Intellectual property.
- Gordon-Bell Prize for development of boundary-element methods for analyzing particle motion during fluid flow.

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Modeling and Predicting Stresses in Thermoset Materials

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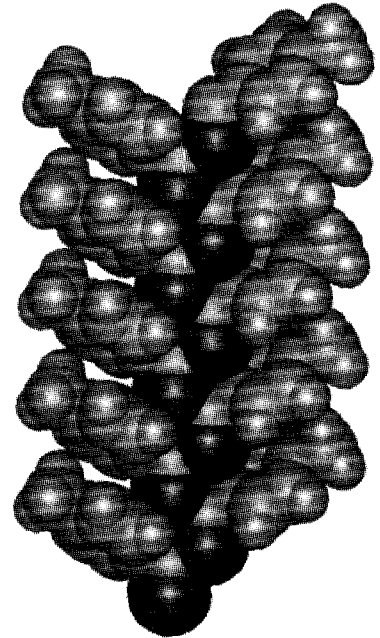
Sandia National Laboratories offers specialized expertise in modeling and predicting stresses in thermoset materials:

- Fully three-dimensional, finite-element modeling capability for analyzing the curing process in low-molecular-weight resins and condensation-type reactions (including epoxies used in encapsulation).
- Cure modeling validated to within 10% of actual performance.
- Thermal chemical code to predict reaction rate, exotherms, and heat transfer associated with cross-linking reaction. Results are passed on to a structural code, which computes the cure-shrinkage and accompanying evolution in viscoelastic properties needed to predict the deformations and stresses generated during cure. Urethanes and polyesters would also be relevant in applying the model.
- Nonlinear viscoelasticity modeling capability to predict dimensional stability, physical aging, and stresses through yield in polymers. Nonlinear viscoelasticity represents an advancement to cure modeling and compliments it. Nonlinear viscoelasticity can be used for analyzing the nonlinear thermoviscoelastic deformations and stresses in polymers subjected to arbitrary loading histories.

Both modeling approaches are made possible by the massively parallel teraflops computer and by proprietary three-dimensional, finite-element analysis codes. Sandia has the facilities to characterize time-temperature-reaction dependent viscoelastic properties of polymers and predict yielding in shear, compression, tension, and combined loadings.

Applications

- Electronic packaging.
- Composite materials.
- Adhesively bonded joints.
- Encapsulation of PCBs and electrical components.
- Dimensional stability of polymers.
- Automotive paints.
- Physical and chemical aging and dimensional stability of polymers.
- Developing failure models.



Potential Benefits

- Modular software and iterative-solution algorithms make complex, three-dimensional analysis practical.
- Diagnosis of performance characteristics with recommended changes in process to improve performance.
- Shortened cure schedules.
- Optimized stresses, warpage, and deformations using analysis to tailor process parameters (temperature, time) a priori.
- Reduced number of proof tests needed, shortened time-to-market, and improved quality and reliability.



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- True process modeling of parameters affecting end product.
- Accurate prediction of stresses for failure models and prediction of dispersive waves in shock propagation problems.

Demonstrated Achievements

Reduced development time on defense components by 50%.

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Computer Modeling of Polymeric Materials

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Sandia National Laboratories capabilities:

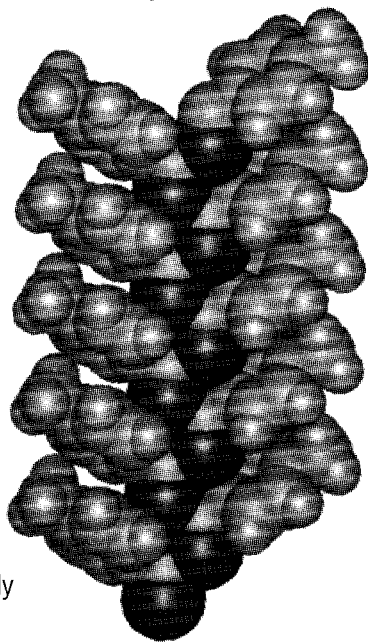
- Predicting macroscopic properties and miscibility characteristics of polymer liquids and polymer alloys from a knowledge of the molecular architecture of the polymer constituents.
- Predicting equilibrium properties (solubility, adhesion, X-ray defraction, etc.) using the PRISM theory, developed and continually advanced at Sandia and based on proprietary dynamic codes run on massively parallel computers with demonstrated calculations in the tereflop range.

Applications

- Molecular design of new polymer alloys.
- Computer models of synthetic efforts to control polymer architecture through new metalloce catalysts.
- Polymer blends of commodity polymers (polyolefins).
- Gas solubilities models in polymers.
- Polymers near interfaces.

Potential Benefits

Sandia offers the most current technology and the best understanding and experience in applying PRISM to the development of polymers with significantly improved properties.



Although the PRISM theory is commercially available, taking advantage of Sandia's in-depth services is the most effective and productive method of applying the theory to reduce polymer synthesis development time. Sandia's in-depth services include the flexibility to tailor PRISM calculations to meet special customer needs.

Demonstrated Achievements

- Sandia successfully predicted the miscibility and phase behavior of a range of polyolefin blends, as well as the solubility and diffusion of gases in a range of polymers.
- Several major corporate research organizations are implementing the initial modeling software to develop advanced products.

References

- More than 50 publications and 30 invited presentations at national meetings and universities on PRISM modeling and theory.
- 1992 R&D 100 Award for PRISM.
- 1996 DOE Basic Energy Sciences award for excellence in Materials Chemistry for PRISM theory.

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Molecular Simulation of Polymeric Materials

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Sandia National Laboratories can predict mechanical, transport, and interfacial properties of polymers, based on our knowledge of the molecular architecture of monomers and our proprietary molecular simulation codes that run on massively parallel teraflops computers and involve up to 1 million atoms.

Applications

- Molecular design of high-barrier films.
- Polymer membranes for gas separations.
- More durable aging-resistant rubbers.
- Predictions of strength properties of polymer materials and polymer surfaces, gas diffusion rates through barrier films, and rate-of-strength loss due to oxidation.

Potential Benefits

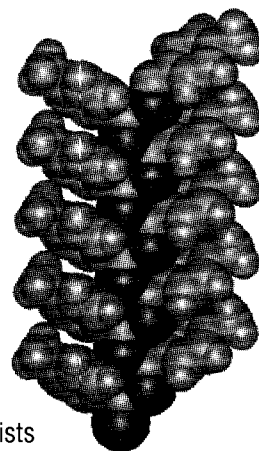
- Molecular simulations with up to 1,000,000 atoms, which result in more reliable predictability of polymer properties compared with the 100,000 or less atoms used in competitive modeling systems. The unique, massively parallel computers at Sandia enable calculations at this order of magnitude.
- Direct observation of a molecular architecture's impact on the macroscopic properties of polymers identifies cause-and-effect relationship between chemical structure and final properties and creates critical benchmarks for performance attributes.
- Low-cost "what-if" computer experiments to screen candidates for enhanced performance products.

Demonstrated Achievements

- Successfully predicted the diffusion of oxygen in polyisobutylene, ethylene-propylene rubber, polyethylene, and polypropylene.
- Generated realistic cross-linked polymer structures containing more than 1,000,000 atoms and exceeding 0.01 microns in size.
- Simulated gradient-driven flux rate of penetrant molecules through polymer membranes.

References

The polymer simulation capability at Sandia is part of a 3-million-dollar research program in polymer degradation. This program supports work in a variety of disciplines, including experimental studies and engineering models. Sandia scientists working in this field have extensive experience in materials modeling on the atomic scale.



Sandia has issued 16 polymer simulation publications and has participated in numerous conferences, including several "invited seminars."

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Adhesion Studies

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Sandia National Laboratories is conducting leading-edge studies of adhesion and associated interfacial issues in actual bonding for manufacturing and research applications. These studies involve modeling and fracture mechanics in conjunction with fundamental adhesion/interface studies to understand the nature of the adhesive bond.

Sandia has developed finite-element code to predict adhesion failure. Some of our equipment and techniques includes contact mechanics apparatus, dynamic and static contact-angle equipment, fracture mechanics measurement techniques, imaging apparatus with micron-level and 30-frames/sec recording capabilities, techniques for measuring highly filled polymer flow and cure in thin-gap (10-micron) structures, dynamic mechanical analyzer, and thermal analysis techniques.

Applications

- Electronic packaging/underfill industry.
- Adhesives, encapsulants, and sealant formulators.
- Bonding applications in general manufacturing.
- Polymers with high-modulus materials such as metals.

Potential Benefits

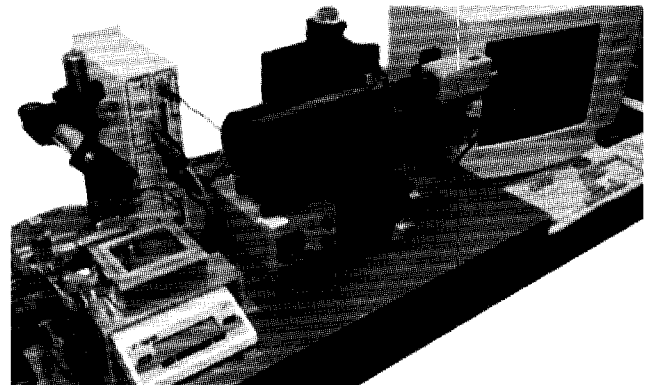
- New adhesives with enduring, reliable interface via a fundamental understanding of the interphase region and material curing.
- Improved understanding of behavior requirements of highly filled epoxies used in flip chip underfill by the packaging industry.

Demonstrated Achievements

- Developed tools for characterizing flow of underfill materials and for testing adhesive joints at an electronics packaging manufacturer.
- Led a nation-wide team in the development, testing, and specification of lead-free polysulfide sealant replacements.

References

Invited participant in DoD, SAE G8 and G9, coating and sealing groups, SEMATECH Liquid Encapsulation Program, Minnowbrook Conference.



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Flip Chip Underfill Studies

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Sandia National Laboratories has conducted leading-edge studies of the flow of flip chip underfill materials and developed simple tools to characterize flow properties.

Sandia offers—

- Significant expertise in understanding adhesive systems and in actual bonding for manufacturing and research applications.
- Modeling and proprietary codes in conjunction with fundamental encapsulation studies to understand the nature of encapsulant filling, cure, and internal stress generation.
- Contact mechanics apparatus, dynamic- and static-contact-angle equipment, fracture mechanics measurement techniques, imaging apparatus with micron-level and 30-frames/sec recording capabilities, techniques for measuring highly filled polymer flow and cure in thin-gap (10 microns) structures, dynamic mechanical analyzer, thermal analysis techniques.
- PC-based model for use by formulators and process engineers in working on processes.

Applications

- Electronic packaging/underfill (flip chip).
- Materials formulators.

Potential Benefits

An improved understanding of the behavior of highly filled epoxy flow in 10-100 micron gaps is required to meet the conflicting materials requirements necessary for an effective underfill. Sandia expertise is the key to shorter product

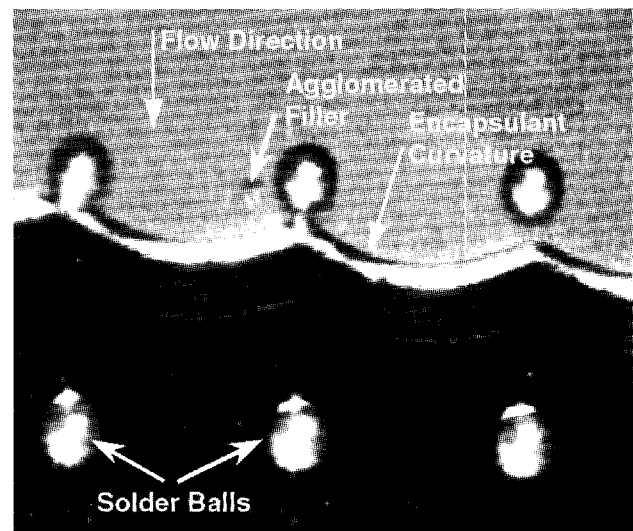
development time, as our track record in product development proves.

Demonstrated Achievements

- Developed tools for SEMATECH for characterizing flow of underfill materials.
- Developed imaging system for viewing the flow during underfill.

References

Invited participant at SEMATECH Liquid Encapsulation Program, Minnowbrook Conference.



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Unique Characterization Tools for Measuring Physical and Chemical Aging of Polymeric Materials

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Sandia offers a proprietary suite of characterization tools for studying and understanding aging phenomena in polymeric materials.

Optical Characterization

- Leading-edge optical characterization of polymeric materials for structure/composition determination, quality control, and application suitability.
- Thin-film/surface light scattering instrumentation and proprietary numerical code.
- Custom prism coupler refractometer and analysis code.
- Time-resolved absorption and emission instrumentation.
- Thin-film optical waveguide characterization and numerical code.

Modulus Profiling

- Mapping of modulus measurements across the polished cross-section of polymeric materials with approximately 50-micrometer resolution using a unique proprietary instrument.
- Scaleable to 5 micrometers.
- Margin of error of $\pm 5\%$ compared to macro-modulus analytical techniques with error rates of 20 to 30%.

Composition Profiling

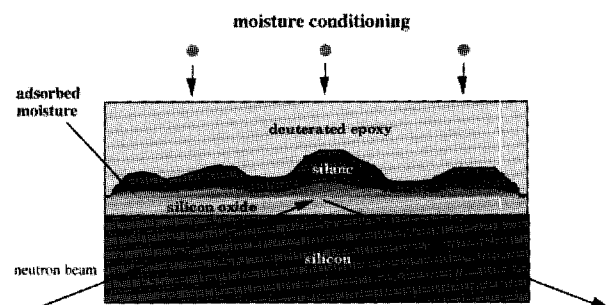
- Neutron reflection for determining the concentration depth profile of individual species, such as water, through thin organic films, or for determining the presence of contaminant layers on solid surfaces.

- Access to neutron scattering facilities and expertise in neutron reflection, deuterium labeling, and moisture profiling.
- Thicknesses in the range of 5 to 2000 angstroms can be examined. Composition profiles can be obtained at buried interfaces in-situ.

Applications

- Optical application of transparent, thin-film polymeric materials such as waveguide materials, clear-coats for painted surfaces, and nonlinear optical polymeric materials.
- QC in microelectronics thin-film processes.
- Investigation of grain boundaries in semiconductors.
- Studying cure state, uniformity of cure, and aging of elastomeric materials.
- Identifying and quantifying diffusion-limited oxidation effects affecting accelerated aging.
- Paint coatings, engineering polymers, rubber compounds.
- Understanding the mechanisms of adhesive failure and the corrosion-resistant properties of organic films.

Moisture uptake at SiO_2 /silane/epoxy interface by neutron reflectivity



Composition profiles can be determined with 5-Å resolution normal to the interface.



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Potential Benefits

- Optimization of polymeric and organic materials in demanding optical applications via detailed characterization of optical behavior.
- Correlation of scattering data to actual physical effects.
- Better understanding, preparation, and aging of polymers.
- Improved methods of predicting polymeric lifetimes from accelerated aging experiments, thereby improving the selection and development of new materials with significantly improved performance.
- Improved organic coatings for adhesion and corrosion resistance.

Demonstrated Achievements

- Thin-film optical characterization techniques using ferroelectric thin-films and polymeric thin-films.
- Favorably impacted product development of a major Fortune 500 company as a result of breakthroughs in understanding of previously unknown aging phenomena.
- Interfacial moisture profiles obtained through thin epoxy films on silicon and in polyurethane films on metals. In each case, the water profile was obtained as a function of surface chemical treatment.

References

- Invited speaker at Materials Research Society Meetings.
- Numerous publications (including *Trends in Polymer Science*, Service Life Prediction Symposium) on aging effects for polymers in thermal and radiation environments.
- Keynote speaker at Elastomer-Service Life Prediction Symposium '97.
- Publications in *Journal of Material Science*, *Materials Research Society Symposium Process*, *Journal of Adhesion*, *Journal of Chem. Physics*, *Macromolecules*, *Physics Review Letters*.

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Tunable Infrared-Laser Diagnostics

Organic Materials Program

Sandia National Laboratories offers

- Extensive experience in the development of laser diagnostic methods for characterizing molecular species (hydrocarbons, CO, CO₂, NH₃, NO_x), with a particular specialty in real-time, on-line measurement in production-environment applications.
- A unique system for micro- and macro-scale spectral imaging of condensed-phase materials.
- Extensive tunable infrared-laser facilities at Sandia/California for gas-phase characterization.

Applications

- Detecting contaminants in component fabrication processes.
- Characterizing chemical changes induced by polymer aging.
- Replacing batch/off-line testing with on-line process control in steel and glass manufacturing.

Potential Benefits

- Real-time imaging of chemical species applied to product development and manufacturing processes.
- In-situ measuring of gas-phase species down to trace levels during aging and reliability studies.
- Real-time monitoring of off-gas streams for industrial process control.

Demonstrated Achievements

- Demonstrated a differential imaging system for visualizing solvent and contaminant distribution on surfaces by laser illumination.
- Developed a tunable infrared-laser system for measuring chemical aging effects in polymers with diffraction-limited spatial resolution (6μm).

- Developed an off-gas sensor for real-time process control in the harsh industrial environment of a steel mill.

References

- Two patent applications filed.
- Publications in *Applied Spectroscopy* and diverse conference proceedings.
- Cooperative programs between Center for Materials Research and Combustion Research Facility.
- Several projects underway with U.S. industrial partners and government agencies.

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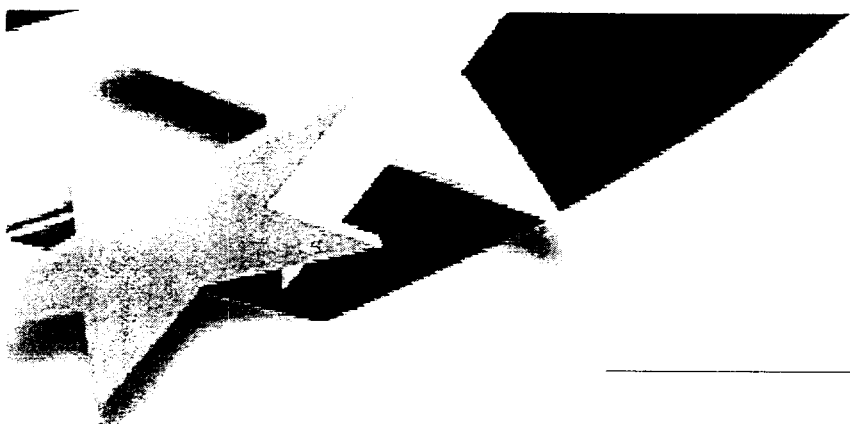


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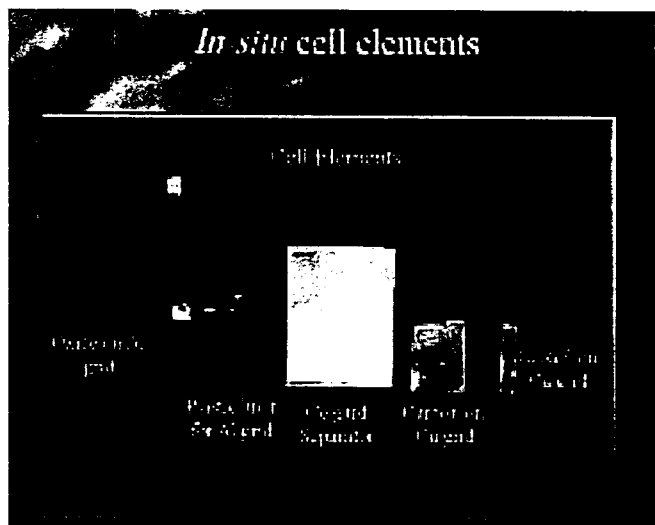
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High-Capacity Carbon for Li Rechargeable Batteries

Sandia National Laboratories is developing advanced carbon materials for rechargeable batteries that improve performance and cycle life.

Specifically, carbon anodes have become the material of choice for lithium ion rechargeable batteries since carbon anodes offer improved safety and performance compared to lithium metal anodes.



Sandia understands the fundamental physical and chemical phenomena that dictate the performance of anode materials. Consequently, we have developed and exploited the capability of tailoring carbon materials for electrochemical applications.

Materials R & D at Sandia National Laboratories is world-class. Sandia capitalizes on its unique analytical methods (NMR and in-situ XRD, for example) that allow evaluation of materials interactions and phenomena in battery systems.

Applications

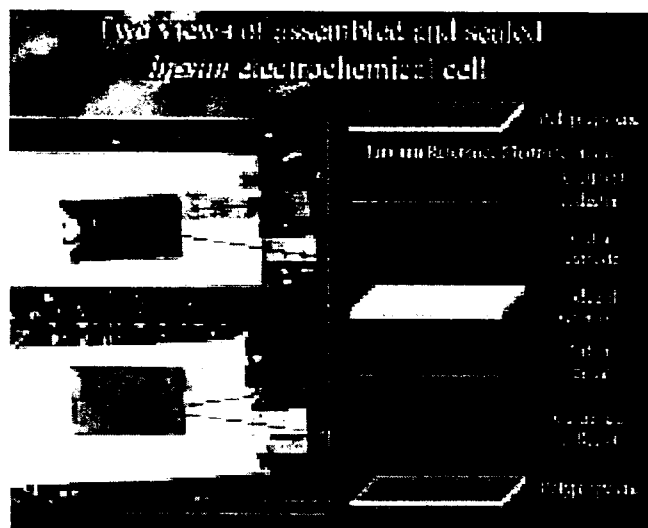
The rechargeable battery industry for portable electronics in the U.S. is projected to be \$8 billion/year by 2000 (up from \$6 billion in 1997). Any rechargeable battery manufacturers or chemical/material manufacturers that plan to supply materials to the battery industry would benefit from Sandia's experience in advanced carbon materials.

Potential Benefits

Better battery performance in regards to higher energy density, higher rate capabilities, and longer run times.

Demonstrated Achievements

We have demonstrated very high capacity carbon material development—up to 600 mAh/gram under certain charging conditions.



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References

- More than 12 publications with 1 patent issued and 1 in application.
- Sandia-developed collaborations with the U.S. battery industry (including Eveready Battery Corporation, Rayovac, Wilson Greatbatch Ltd., as well as USABC Contractors) and material suppliers (such as Dow Corning Corporation).
- More than \$11 million invested by Sandia in industry-funded work specifically on carbon material development and characterization.
- Sandia-organized professional society symposia on battery materials. Sandia was lead organizer of two MRS Symposium on "Materials for Electrochemical Energy Storage and Conversion - Batteries, Capacitors and Fuel Cells," and editor of the MRS Proc. Volumes 393 (1995) and 496 (1998).

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Battery Materials and Performance

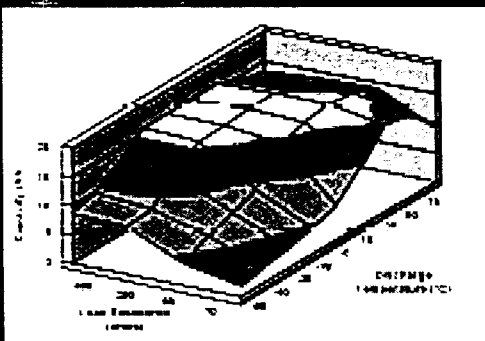
Sandia National Laboratories offers unique modeling and electrochemical characterization capabilities for the advancement and understanding of battery materials and performance:

- Sandia's modeling of battery performance employs an integrated approach that involves first principles, artificial neural networks (ANN), and electronic circuit emulation software (PSPICE), which delivers greater power and flexibility than any of the elements separately.

This unique capability is unmatched by other labs or universities which possess elements of this approach as a "stand-alone" capability.

The power of the integrated approach allows Sandia to numerically simulate complex phenomena that are not easily solved by other approaches and to link battery design and material properties with application electrical requirements.

Capacity Delivered From a Battery Depends on the Temperature and Load Characteristics



- Characterization of advanced materials for electrochemical devices is difficult to do in a meaningful way. Sandia has extensive experience in evaluating these materials and can provide cost-effective quality analyses of performance and usefulness in battery applications.

Expertise at electrochemical evaluation is driven by defense applications where knowledge of how electrochemical devices and constitutive materials behave is an important requirement.

A core Sandia competency is the understanding of battery performance fundamentals under normal and abnormal use conditions.

Sandia has developed standard methods of analysis and has attained an excellent grasp of what makes advanced materials useful in commercial applications.

- World-class test equipment, some of which is unique to Sandia, and a well-developed infrastructure for analysis of battery and fuel cell materials are outgrowths of our defense programs and are available to help solve material development problems in the commercial power source field.

Applications

- Chemical and advanced materials companies.
- Battery manufacturing companies.
- Integrated electronics companies seeking to optimize power solutions.

Batteries not well suited to the power requirements of the application can be very inefficient and fail prematurely. An intelligent modeling approach and electrochemical characterization allows the matching of battery design to the target application in a way that enhances the performance of the entire system.



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Potential Benefits

Battery Modeling

- Longer life and better performance in any battery-powered electronic device.
- More efficient (faster, lower cost) and accurate selection of optimum battery chemistry for a specific application.
- Ability to focus battery improvement in areas with the most potential benefit.

Electrochemical Characterization

The success of improved battery and power source technology will depend on advanced materials as well as on developing an in-depth understanding of existing materials and material interactions. The benefit will be increased efficiency, better performance of batteries and fuel cells, as well as the potential of lower cost.

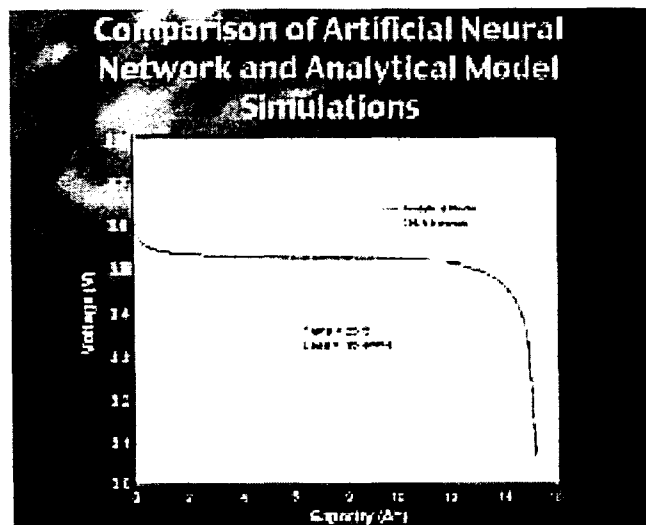
Sandia provides confidential analyses for customers, often including a comparison of their samples to performance obtained on widely available commercial materials. Material suppliers often desire to have analyses done by a third party with expertise in the field of use (power sources in this case), provided the results are kept proprietary.

Demonstrated Achievements

Battery Modeling

Sandia National Laboratories has applied battery modeling expertise to improve our understanding of lithium/thionyl chloride battery performance. Modeling was part of a program that successfully demonstrated a concept for long life (> 5 yr.) under a very wide temperature range (-40°C to +65°C).

Sandia has used the first-principles approach to prepare "training data sets" for the ANN that would have been extremely time-consuming and equipment use intensive to obtain experimentally, and the simulation of electrode passivation was modeled by ANN in the absence of available analytical expressions. Sandia has a major initiative in



numerical modeling funded by DOE—Accelerated Scientific Computing Initiative (ASCI)—and has invested substantial effort to develop battery performance modeling for defense applications that require high-reliability, long-life power sources.

Electrochemical Characterization

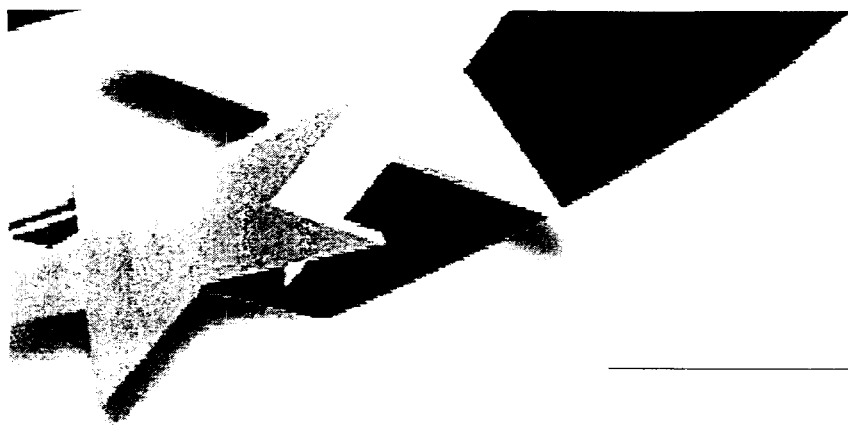
Sandia has worked with several material companies on a contract basis to evaluate their materials. Customers include chemical manufacturers (Dow Corning) and polymer companies (Solvay and Elf Atochem), as well as others that have asked to remain confidential.

References

- Sandia has written more than 40 publications and has presented work at 3 international meetings in the fields of battery modeling and electrochemical characterization.
- Sandia is developing a licensing framework arrangement with the University of South Carolina, a collaborator in the first principles model.
- Sandia was the lead organizer of two MRS Symposium on "Materials for Electrochemical Energy Storage and Conversion - Batteries, Capacitors and Fuel Cells," and editor of the MRS Proc. Volumes 393 (1995) and 496 (1998).

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Chiral Molecular Recognition and Catalysis

Sandia National Laboratories offers computer-guided synthesis of molecular receptors for chiral chemical species. To guide the synthesis of metalloporphyrin-based superstructures capable of specifically binding chiral chemicals and biochemicals, Sandia uses proprietary molecular simulations and normal-coordinate structural analyses, which include a Sandia-developed force field for organometallics and normal-coordinate structural decomposition procedures. The synthesized chiral receptors are then characterized using resonance Raman, NMR, UV-visible absorption, CD, mass-spec, X-ray structure, and chemical reactivity studies.

Sandia's level of expertise in porphyrin synthesis, experimental characterization, and molecular structural analysis of the receptors and receptor complexes is unrivaled, with more than 20 years of experience in porphyrins and related compounds and resonance Raman spectroscopy and theory. Sandia has more than 12 years' experience in molecular modeling and molecular design and more than a decade of experience in catalysis and photochemistry.

Applications

- Chiral catalysis and separations, and chemical and biochemical sensing.
- Control of living polymers and polymer tacticity.
- Optical chiral chemical sensors for biomedical, CBW, and chemical manufacturing applications.
- Catalysts for enantioselective synthesis of chemicals and polymers.
- Photochiroptical materials.

Potential Benefits

Sandia National Laboratories' chiral modeling and synthesis expertise can help the pharmaceutical, insecticide, pesticide, and polymer development and manufacturing industries experience shorter product development times and increase the return on their R&D investment.

In addition, Sandia can help these industries develop and evaluate uniquely different classes of molecules aimed at sensing and catalysis.

Demonstrated Achievements

Two new types of chiral porphyrins for molecular recognition of chiral compounds have been demonstrated:

- One is a chiral porphyrin that makes a large conformational change between an open and closed geometry (flytrap) in response to coordination of a specified molecule (fly).
- The other is a designed chiral porphyrin containing no chiral atom.

The chirality is induced by the strong steric constraints built into the molecule. Strategically placed hydrogen-bonding groups provide high enantioselectivity for the targeted chiral amine as shown by proton NMR measurements. This prototypical receptor is the first to be fully computationally designed, synthesized, and experimentally validated.

The porphyrins have optical properties that make them good reporting groups for sensing the binding event. They also have highly variable structures that can be adjusted for detecting many interesting chemicals and biochemicals.



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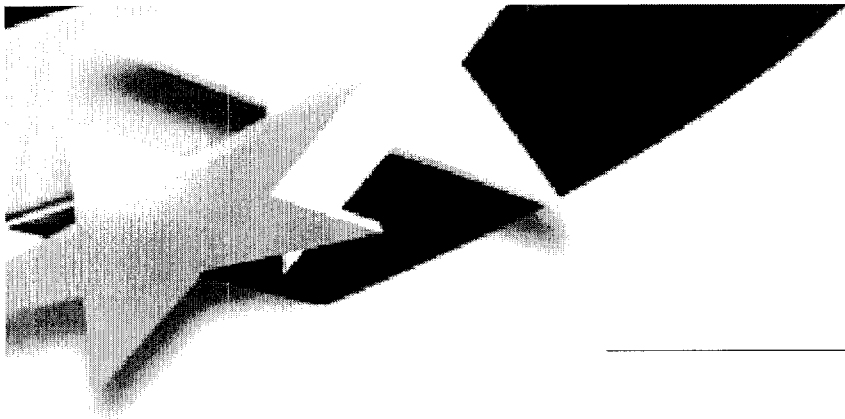
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References

- Two patents issued and 2 pending applications.
- More than 140 papers in refereed journals, and more than 40 other reports issued.
- Attended and participated in more than 400 seminars, with 15 chairmanships at symposia.
- One book currently in preparation. Most recent in chiral recognition and catalysis: *A Pyridine-Sensitive Venus Flytrap Porphyrin*, M. Mazzanti, J. C. Marchon, M. Shang, W. R. Scheidt, S. L. Jia, J. A. Shelnutt.
- *J. Am. Chem. Soc.* 1997, 119, 12400-12401. "Optical Reporter Groups for Sensing Chiral Chemicals," J. A. Shelnutt, C. M. Muzzi, S. L. Jia, C. J. Medforth, K. M. Smith, J. Zhang, Y. Qiu, 7th International Meeting on Chemical Sensors, Beijing, China, July 27-30, 1998.

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Improved Oxygen Reduction Electrocatalysts

Sandia National Laboratories has developed non-precious metal fuel cell cathode electrocatalysts for improved oxygen reduction.

Sandia has demonstrated its expertise in computer-aided molecular design (CAMD) and structure optimization of electrocatalysts, which are designed macrocycles with steric pockets to enhance oxygen binding. Synthesis and testing are integrally coupled to the design efforts for iterative improvements in design. Sandia has shown significant depth and leveraging of CAMD and macrocycle design, synthesis, and testing.

Applications

- Fuel cells
- Sensors
- Batteries
- Biomedical
- Pharmaceutical design

Potential Benefits

- New and improved low-temperature PEM and alkaline fuel cells.
- Improved performance of cathode kinetics, which translates directly into improved system efficiency.
- Lower costs because of the use of non-precious metal electrocatalysts.

Demonstrated Achievements

Demonstrated first-generation electrocatalysts simply wetted onto porous carbon electrodes for performance testing. Next generation will likely incorporate designs permitting covalent attachment to electrode surface for enhanced performance and longer-term testing.

References

Several patents and more than 10 publications issued on designed metalloporphyrins.

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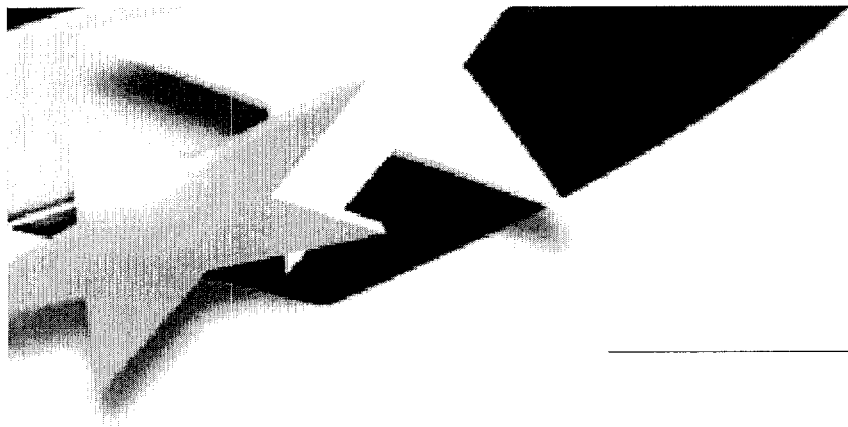


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Inorganic Thin Films

Inorganic thin films based in zeolitic materials are being developed as advanced membranes for chemical feedstock and light gas separations.

Sandia National Laboratories has demonstrated:

- The growth of oriented zeolite thin films on porous supports
- New zeolite phases with adjustable porosity
- New chiral zeolitic phases using a multidisciplinary approach combining high-performance computational modeling and simulation of porous materials and pore diffusion coupled with unique expertise in synthesis and growth of novel zeolite thin films on porous supports
- The capability to test and validate performance for a wide range of separations
- The ability to leverage expertise in sol-gel chemistry and thin film deposition
- High-performance computing capabilities

Applications

Chemical, refining, pharmaceutical industries.

Potential Benefits

- New products
- Improved processes
- Opportunities for direct coupling of separations to high-temperature processes
- Energy savings
- Chemical waste avoidance

Demonstrated Achievements

- Modeling and simulation of light gas molecular diffusion through a variety of porous materials.
- New oriented zeolite thin films and novel defect-free zeolite/sol-gel composite thin films.
- Versatile synthetic approach to porous inorganic membranes.
- New tailored zinc phosphate zeolite phases with adjustable pore sizes
- Newly characterized chiral zeolite phases.

References

- Several patent disclosures and several preprints for journal publications.
- Cooperative Research and Development Agreement (CRADA) with Amoco Chemical for chemical feedstock separations.
- Sandia chaired a special symposium on Catalysis with Designed Materials at an ACS Fall meeting.

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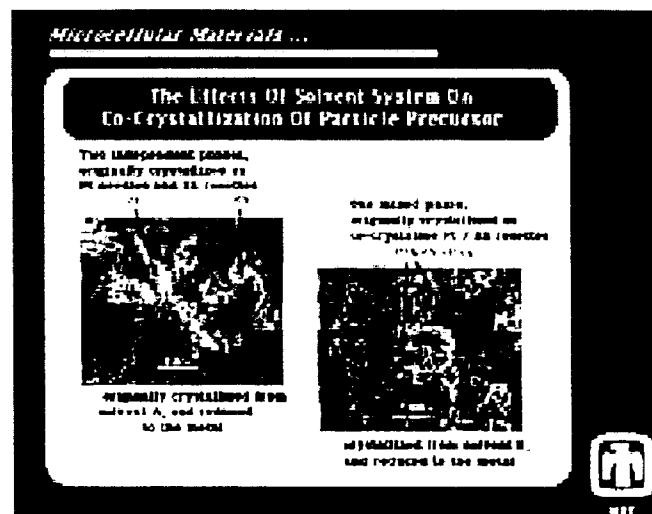


Ultra Pure Small Particles / Noble Metal Properties: Metals and Alloys

Sandia National Laboratories offers unique processes, capabilities, and experience in producing small noble metal particles (50-500Å). Sandia can produce these particles as high purity metals or as alloys. Variations of this process are applicable also to nonmetals, either organic or inorganic materials.

The particles are "assembled" rather than attrited, thus ensuring high purity and clean, reactive surfaces. An extension of the process has successfully integrated the placement of the particles on substrates as part of the synthetic process. This allows the production of highly loaded catalytic supports within a single-step process.

Sandia, under the auspices of its Microcellular Materials R&D Program, has worked more than 10 years tailoring properties of low-density materials and powders to meet the performance needs of defense-related programs. The common thread throughout this work has been "Materials Micro-Engineering By Design," that is, applying a

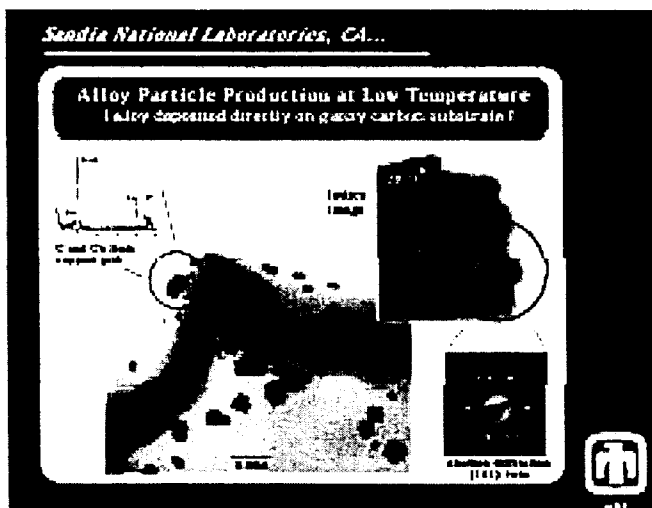


fundamental materials understanding of solution thermodynamics (like free energy of mixing) to select a favored particle morphology outcome.

The breadth of Sandia National Laboratories' experience is unparalleled and allows access to understanding of and experience with peptides to polymers, from salts to ceramics, from organics to refractory metals.

Applications

- Chemical companies and companies in the petroleum industry with an interest in catalysts for processing, synthesis, and energy-related applications.
- Powders used in coatings, thick-film lithography, identification tags, and drugs, with particular emphasis on high-temperature applications, the microelectronics industry, and pharmacology.



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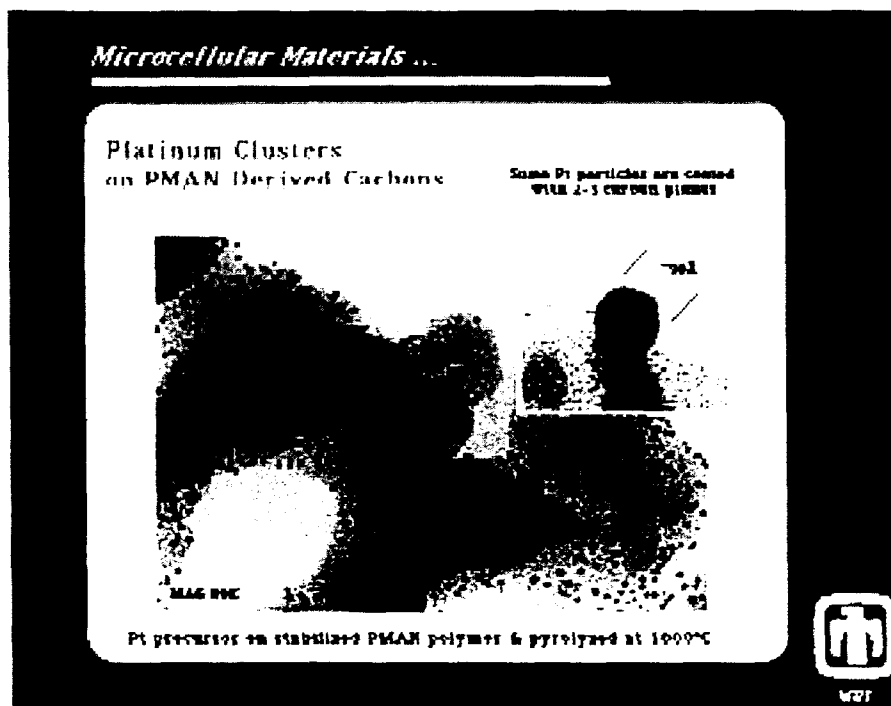
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Potential Benefits

Sandia offers a "virtual laboratory"—an interdisciplinary team of scientists and engineers both in-house and via connections across the entire DOE laboratory system and associated universities. On site, elaborate characterization capabilities provide both complete and timely analyses for real-time experimental feedback. The most likely benefits lie in high-value-added applications, either where other methods fail to meet the performance specification or where the technology is enabling a whole new, as yet untapped, arena. Such an example would be drug inhalation therapy.



Demonstrated Achievements

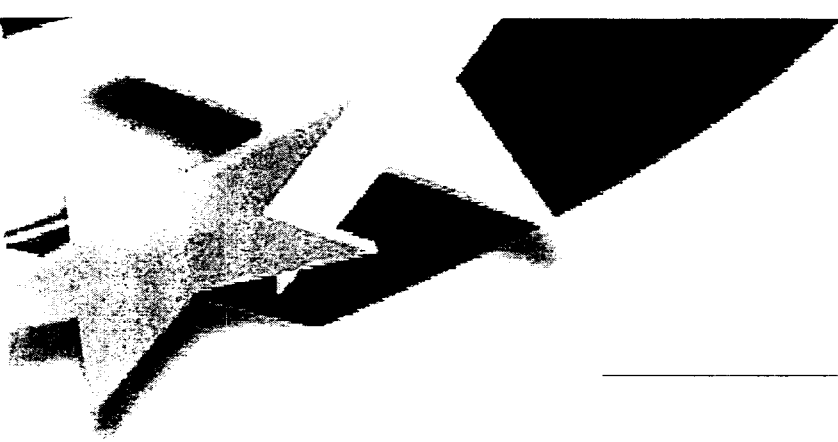
- Sandia National Laboratories has completed 50 man-years of R&D related to the engineering of microcellular materials. Sandia also has an enduring basic research program in this area and has partnered with many companies and universities, both academically and commercially, to provide tailored materials. This knowledge base provides a considerable technical leverage to new customers.
- Three Industrial Cooperative Research and Development Agreements (CRADAs) have been executed.

References

- Two patent applications are being filed.
- Several alliances with universities, industry, and other national labs have been established and several publications issued.

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Plasma Processing of Materials

Sandia National Laboratories offers multifaceted programs for studying plasma alterations of surface properties via deposition, cleaning, chemical functionalization, and plasma-modeling capabilities for process development and control.

Sandia has developed unique and powerful research tools that include molecular-beam plasma-probing techniques for addressing plasma chemistry and fiber optic-based sensors for measuring gas-film interactions.

Sandia has demonstrated experience with plasma deposition of a wide range of ceramic, metallic, and polymeric materials (including silicon nitride and oxide, tungsten, polystyrene, vinylpyridine, allyl sulfides, fluorocarbons, allyl amine, and methylmethacrylates).

Sandia also employs unique molecular-beam probes of plasma chemistry, laser *in situ* plasma diagnostics, fiber-optic characterization of plasma-polymer swelling behavior, and proprietary detailed plasma modeling capabilities (0-D through 3-D codes) with elaborate gas and surface chemistry mechanisms and fluid mechanics. Supporting these unique capabilities is experience in large area coatings using shaped electrodes and nano-particle synthesis in plasmas.

Applications

Industries with an interest in —

- Altering the surface properties of materials to develop new products and/or enhance performance in areas such as

semipermeable membranes, barrier coatings, and chemical sensors.

- Applying techniques for addressing plasma and surface chemistries, including sensor methods for measuring gas diffusion and solubility in plasma-polymerized films.

Potential Benefits

Companies will benefit from Sandia National Laboratories' ability to assemble experienced teams of people with unique skills aimed at providing synthesis and modeling, *in situ* probe analysis, system prototyping, and physical demonstrations-of-concept in plasma processing of materials for developing novel products or products with improved characteristics.

Demonstrated Achievements

- Developed a new volatile organic compounds (VOC) sensor based on plasma-polymerized film that substantially reduced the cost of in-field monitoring while improving monitoring coverage.
- Developed plasma coating to promote metal-polymer adhesion aimed at improving the life of composite materials for a large U.S. company.
- Performed first direct measurement of plasma-generated radical reaction rates at surfaces (SiH, NH, SiO, and OH radicals) that enabled the development of a mechanism for plasma deposition in the microelectronics industry.



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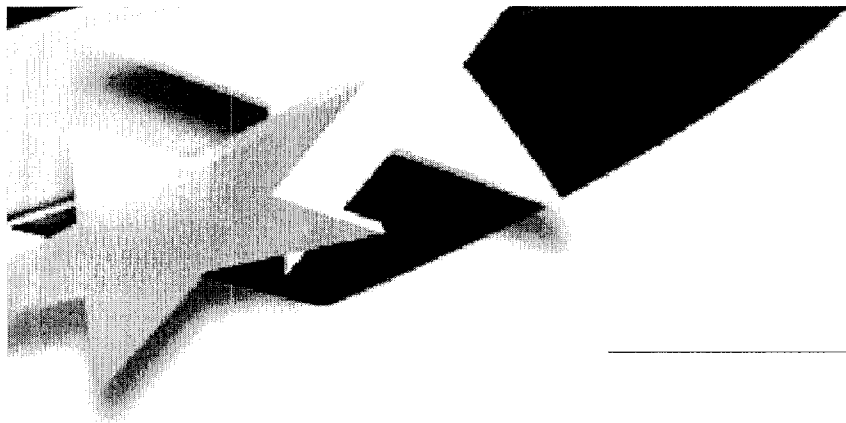
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References

- Patented technique for synthesizing nano-particle materials.
- More than 25 papers presented at national symposia and more than 15 peer-reviewed papers published in the preceding 5 years.

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Micro-porous Carbon Foams

Sandia National Laboratories' specialized expertise in polymer chemistry and macromolecular physics spans a wide range of materials applications to yield microcellular materials and their derivatives, engineered to provide unique performance advantages. Sandia's computational tools include proprietary code developed to predict performance (such as adsorption and transport of two-phase media) in microcellular materials.

Applications

- Energy storage materials devices.
- Filtration and separation.
- Insulation media.
- Low-mass structures.
- Low-temperature alloys via non-abrading methods.
- Powders with unique shapes and properties.
- Stable suspensions for biomedical.
- Low-density foams for immobilizing particulate beds.

Potential Benefits

- Specifically engineered products in lieu of adapting existing products for new applications.
- Custom-tailored properties such as cell size, window size, and composition.

Demonstrated Achievements

- More than 50 man-years' experience dedicated to synthesizing critical new materials for nonnuclear components.
- Two recent Sandia inventions transferred into the

commercial sector within 16 months of conception.

- Four products introduced into the market by two different Fortune 100 companies (including Bethlehem Advanced Materials Corporation) using Sandia's microcellular expertise as an enabling technology in cost-effective solutions for value-added products.

References

- Five patents and 3-4 disclosures being pursued.
- Several Cooperative Research and Development Agreements (CRADAs) and partnerships.
- Publications in MRS, ECS, and ACS proceedings.
- University, industry, and national lab alliances.

For more information

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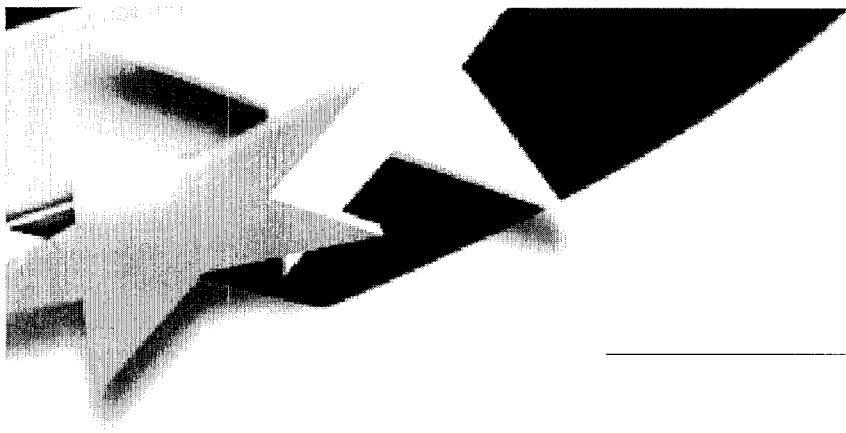


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Micro-Fuel Cells

Sandia National Laboratories is applying its broad experience in materials and catalysis and its unique engineering capabilities to develop novel materials for macro-fuel cells.

Sandia is pioneering the development of silicon-based micro-fuel cells for microelectronics applications. Supporting this effort are Sandia's Integrated Materials Research Laboratory, Compound Semiconductor Research Laboratory, Microelectronics Development Laboratory, and micromachining and semiconductor fabrication processes and facilities.

Sandia is also developing the capability for small (50-W) fuel cell testing and demonstration in customer applications.

Applications

Engineered materials for conventional power-generation and transportation fuel cells, including:

- Proton Exchange Membrane (PEM) fuel cells: electrocatalysts for oxygen electroreduction, organic/inorganic proton conductors, porous carbons, planning stages for advanced manufacturing thrust.
- Phosphoric acid fuel cells: carbon coatings.
- Solid oxide fuel cells: metal/ceramic joining.

Micro-fuel cells using silicon-based semiconductor technology for:

- Portable electronics
- Microelectronic devices
- MicroChemLab
- Battery power source replacements
- Biomedical/implantable devices

Potential Benefits

- New materials for conventional fuel cells that can reduce costs and increase operating efficiency.
- Capability to package an on-chip power source (micro-fuel cell) for microelectronics applications, which are expected to replace batteries and provide reliable, less costly power generation and (where desired) rechargeable electrochemical power and disposable integrated power sources.
- The ability to produce micro-fuel cells using microfabrication techniques versus the conventional pressed-carbon approach is expected to yield similar cost/performance benefits experienced by the semiconductor industry.

Demonstrated Achievements

A novel gas diffusion electrode structure with new membrane support structures has been developed and validated based on the silicon-based microfabrication technology developed and pioneered at Sandia National Laboratories.

References

- Technical Advance filed at Sandia National Laboratories.
- Published paper: "Porous Silicon Gas Diffusion Electrodes," A. Hecht, T. Guilinger, S. Kravitz, G. Ryba, M. Sailor, C. Willan, K. Zavadil, Electrochemical Society Meeting, San Diego, CA, May 1998

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Catalytic Membrane Reactors

Sandia National Laboratories offers:

- Catalysis expertise in preparing hydrous metal oxide-supported catalysts and supported metal nanoclusters in both bulk and thin film forms.
- Separations expertise in amorphous or crystalline (zeolite) inorganic membrane materials with unique molecular sieving capabilities.
- A systems approach to problem solving, which draws on a range of experts in various fields, including computer modeling and simulation, materials synthesis, characterization, testing (including thin films), and process scale-up/prototype fabrication. This systems approach spans the spectrum of research to development to practice.

Supporting this effort are Sandia's unique Combustion Research Facility, Low Energy Electron Diffraction (LEED) Microscopy, and Small Angle X-Ray Scattering Facility (SAXS). A wide range of test (batch and continuous) and

characterization equipment is also available to support programs related to catalyst and separation materials (both bulk and thin film forms).

Applications

Hydrogen generation and/or purification, especially for on-board (vehicle) reforming strategies:

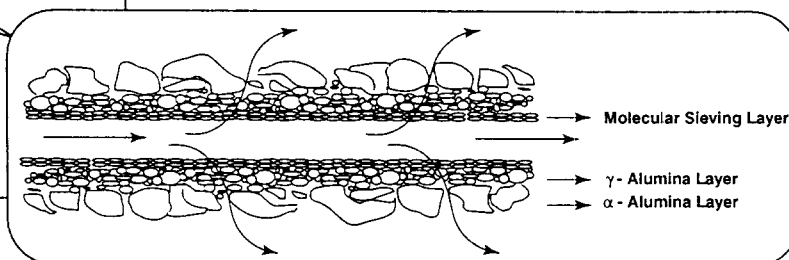
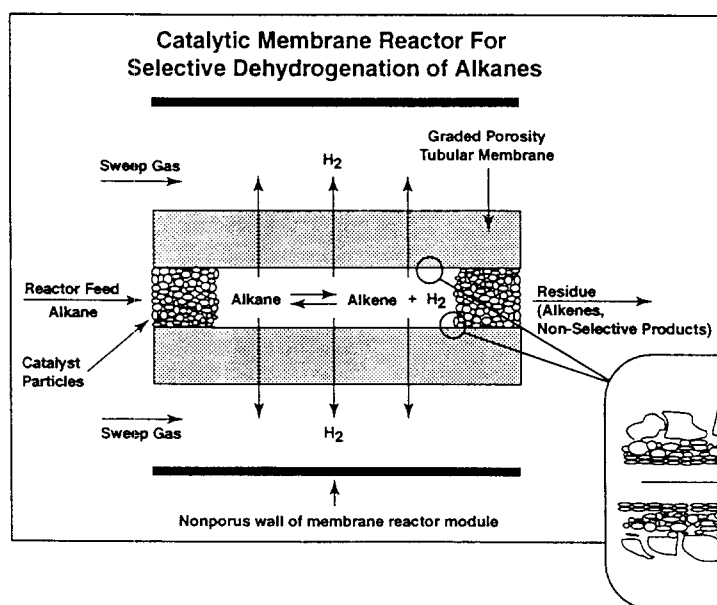
- automotive industry
- petroleum refining
- chemical industry

Potential Benefits

Consistent with future push toward a hydrogen-based economy and global climate change strategies.

Demonstrated Achievements

- Sandia National Laboratories has successfully fabricated full-scale prototype catalytic converters in support of a Cooperative Research and Development Agreement (CRADA) with the Low Emissions Research and Development Partnership, consisting of Ford, GM, and Chrysler (DOE/EE/OTT/OAAT sponsor).
- High activity hydrous metal oxide-supported catalysts have also been developed for coal liquefaction/hydrotreating applications (DOE/FE/FETC sponsor).



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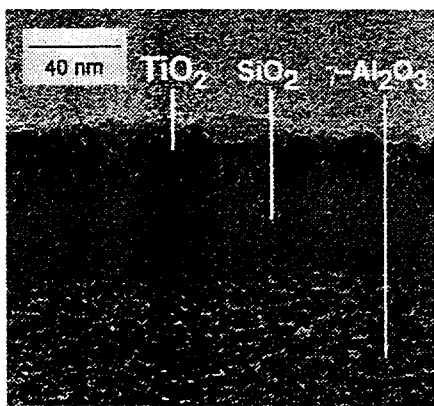


Figure 1

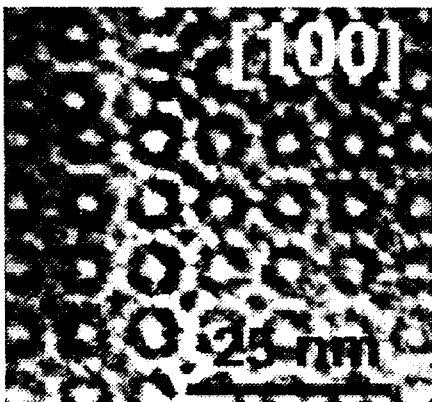


Figure 2

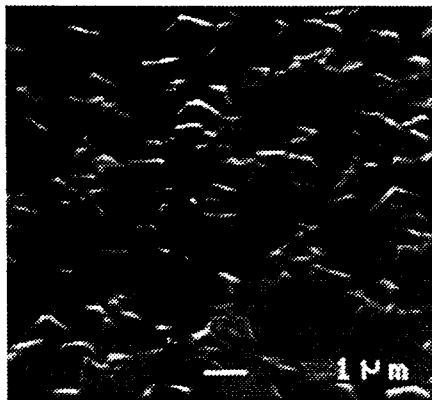


Figure 3



Figure 4

- Minimized weight and volume requirements give catalytic membrane reactors significant advantages in future vehicle applications.

References

- One paper on Catalytic Membrane Reactor Work at 1996 AIChE Annual Meeting.
- Five patents and more than 40 papers on hydrous metal oxide-supported catalyst materials.
- Two patents and more than 10 papers on metal nanocluster catalyst materials.
- Four patents and more than 30 papers on amorphous microporous ceramic membrane materials for separation applications.
- Two patent applications and more than 5 papers on crystalline microporous ceramic membrane materials for separation applications.
- Numerous chaired symposia at national meetings of the American Chemical Society, the American Ceramic Society, and the Materials Research Society.

Figure 1: TEM photomicrograph showing a cross-section view of an HTO/SiO₂ composite membrane deposited on a γ-Al₂O₃-modified alumina tube.

Figure 2: TEM photomicrograph of a surfactant-templated SiO₂ film as viewed along the [100] zone axis. This photomicrograph demonstrates that the material consists of an ordered cubic liquid crystalline mesostructure.

Figure 3: Inorganic thin film membrane – zeolite/sol-gel composite.

Figure 4: Inorganic thin film membrane – zinc phosphate for light gas separations.

For more information

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